

Many-body theory

1 fermion (the easy case)

Basis: $|p\rangle$

P = set of quantum numbers
to represent state

Completeness:

$$\underline{1} = \sum_p |p\rangle \langle p|$$

Orthonormality:

$$\langle p | q \rangle = \delta_{pq}$$

$|p\rangle$ lives in \mathcal{H}_1
 \uparrow
1-body Hilbert space

2 fermions (not too hard)

Basis:

What about $|P\rangle_1 |q\rangle_2$?

$|P\rangle_1$ is in $\mathcal{H}_1^{(1)}$

$|q\rangle_2$ is in $\mathcal{H}_1^{(2)}$

No, states are not antisymmetric
under $1 \leftrightarrow 2$ exchange

$$\text{States } |Pq\rangle_e = \frac{|P\rangle_1 |q\rangle_2 - |q\rangle_1 |P\rangle_2}{\sqrt{2}}$$

are appropriate

Basis of \mathcal{H}_2 is $\{|Pq\rangle\}$

Q: What about $|pq\rangle$ vs $|qp\rangle$?

What about $|pp\rangle$?

More fermions (how it gets hard)

- States in \mathcal{H}_3 have $3! = 6$ individual product states $|p\rangle_1 |q\rangle_2 |r\rangle_3$ per state
- For \mathcal{H}_A , this is $A!$
- Consider evaluating $\langle p_1 \dots p_A | V_{NN} | p'_1 \dots p'_A \rangle_a$ in this way:
 - $(A!)^2$ terms summed up for 1 matrix element
 - Second quantization allows us to efficiently handle antisymmetry
 - also connect between $\mathcal{H}_1, \mathcal{H}_2, \dots$

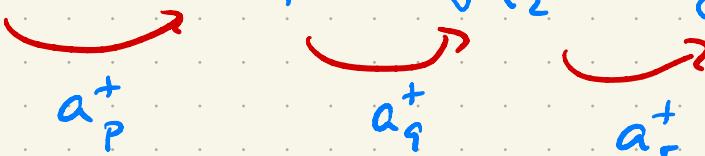
Creation and annihilation operators

Vacuum state $|0\rangle \in \mathcal{H}_0$

→ state with no fermions

Creation operator

$$a_p^+ |0\rangle = |p\rangle \quad \text{create fermion in state } p$$

$$\mathcal{F} = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \mathcal{H}_3 \oplus \dots$$


a_p^+ connects states in different Hilbert spaces

⇒ general Fock space \mathcal{F}
with $\mathcal{H}_0, \mathcal{H}_1, \mathcal{H}_2, \dots$

What about $a_q^+ |p\rangle$?

$$a_q^+ |p\rangle = \begin{cases} |qp\rangle_a & \text{if } q \neq p, \\ 0 & \text{if } q = p \end{cases}$$

Note:
antisymmetrized
state

Cannot have 2 fermions in same state $|p\rangle$!

general case:

$$a_{\lambda}^+ |p_1 \dots p_A \rangle_a = \begin{cases} |p_1 \dots p_A \rangle_a & \text{if } \lambda \text{ not in } \{p_1 \dots p_A\}, \\ 0 & \text{otherwise} \end{cases}$$

very easy to build

antisymmetric A-body product state

$$|p_1 p_2 \dots p_A \rangle_a = a_{p_1}^+ a_{p_2}^+ \dots a_{p_A}^+ |0\rangle$$

\Rightarrow Antisymmetry generated automatically by application of a^+ s.

Product states like this are called "Slater determinants"

Useful properties:

$\rightarrow \mathcal{H}_A$ spanned by basis

$$\left\{ |p_1 \dots p_A \rangle_a \quad \underbrace{p_1 < p_2 < \dots < p_A} \right\}$$

Exercise: Why do we need this?

→ Orthonormality:

$$\langle P_1' P_2' \dots P_A' | P_1 P_2 \dots P_A \rangle_a = \delta_{P_1 P_1'} \delta_{P_2 P_2'} \dots \delta_{P_A P_A'}$$

with $P_1 < P_2 < \dots < P_A$

$$P_1' < P_2' < \dots < P_A'$$

→ Completeness:

$$1 = \sum_{P_1 < P_2 < \dots < P_A} |\langle P_1 P_2 \dots P_A \rangle_a|$$

$$= \frac{1}{A!} \sum_{\substack{P_1, P_2, \dots, P_A \\ \text{unrestricted}}} |\langle P_1 P_2 \dots P_A \rangle_a|$$

→ Antisymmetry:

$$|\langle P_1 P_2 P_3 \dots P_A \rangle_a| = - |\langle P_2 P_1 P_3 \dots P_A \rangle_a|$$

$$\Rightarrow a_{P_1}^+ a_{P_2}^+ |\langle P_3 \dots P_A \rangle_a| = - a_{P_2}^+ a_{P_1}^+ |\langle P_3 \dots P_A \rangle_a|$$

Antisymmetry $\rightarrow a_{P_1}^+ a_{P_2}^+ = - a_{P_2}^+ a_{P_1}^+$

$$\Rightarrow (a_{P_1}^+)^2 = 0, \quad \{a_{P_1}^+, a_{P_2}^+\} = 0 \text{ with anticommutator } \{A, B\} = AB + BA$$

Annihilation operator:

$$a_p |q\rangle = \begin{cases} |0\rangle & \text{if } p=9 \\ 0 & \text{otherwise} \end{cases}$$

$$a_p |q^r\rangle_a = \begin{cases} |r\rangle & \text{if } p=9 \\ -|q\rangle & \text{if } p=r \\ 0 & \text{otherwise} \end{cases}$$

-1 because we must swap q, r :

$$a_p |q^r\rangle_a = a_p (-1) |r^q\rangle_a = -|q\rangle$$

general form:

$$a_\lambda |P_1 P_2 \dots P_A\rangle = \begin{cases} (-1)^{k-1} |P_1 P_2 \dots P_{k-1} P_{k+1} \dots P_A\rangle & \text{if } \lambda = P_k \\ 0 & \text{otherwise} \end{cases}$$

$$\text{Antisymmetry} \rightarrow \{a_p, a_q\} = 0$$

$$\{a_p, a_q^+\} = \delta_{pq}$$

Many-body operators

- Second quantization also allows us to efficiently represent operators for many-body calculations

* One-body operators

$$\hat{O}_i = \sum_{i=1}^A \hat{o}_i$$

each \hat{o}_i acts only
in space of i-th
particle

↑
sum over all A particles

⇒ Goal: representation that is independent of A

General approach

$$\hat{O}_i = \prod \left(\sum_{i=1}^A \hat{o}_i \right) \prod$$

$$= \frac{1}{(A!)^2} \sum_{\substack{p_1 \dots p_A \\ p'_1 \dots p'_A}} |p_1 \dots p_A \rangle \langle p_1 \dots p_A| (\hat{o}_1 + \dots + \hat{o}_A) |p'_1 \dots p'_A \rangle \langle p'_1 \dots p'_A|$$

(*)

(*) For a given Θ_i most particles ($j \neq i$) do not interact $\Rightarrow P_j = P'_j$
 → allows simplification

$$\begin{aligned}\hat{O}_{IB} &= \sum_{P_i, P'_i} \langle P_i | O_i | P'_i \rangle a_{P_i}^+ a_{P'_i} \\ &= \sum_{pq} \underbrace{\langle p | O_i | q \rangle}_{\text{l-body matrix element } O_{pq}} \underbrace{a_p^+ a_q}_{\text{general Fock operators}}\end{aligned}$$

\Rightarrow Expression valid for all A

Consider:

$$\langle \phi' | \hat{O}_{IB} | \phi \rangle \quad |\phi\rangle = |P_1 \dots P_A\rangle$$

$$|\phi'\rangle = |P'_1 \dots P'_A\rangle$$

For one P_i, q

\hat{O}_{IB} connects p in $|\phi\rangle$ with q in $|\phi'\rangle$

$\Rightarrow |\phi\rangle, |\phi'\rangle$ must have same number of particles A

$\Rightarrow |\phi\rangle, |\phi'\rangle$ may only differ by ≤ 1 single particle state ($p \leftrightarrow q$)

Example:

- Particle-number operator

$$\hat{N} = \sum_p a_p^+ a_p$$

for $|\phi\rangle = |p_1 \dots p_A\rangle$

$$- \langle \phi | \hat{N} | \phi \rangle = A$$

$$- \hat{N} | \phi \rangle = A | \phi \rangle$$

Other examples

$$\text{kinetic energy } T = \sum_i \frac{p_i^2}{2m}$$

$$\text{one-body density } \rho = \sum_{pq} a_p^+ a_q$$

* Two-body operators

$$\hat{V}_{2B} = \sum_{i < j=1}^A \hat{V}_{ij}$$

pairwise interactions
between
particles i, j

$$= \frac{1}{2} \sum_{i \neq j=1}^A \hat{V}_{ij}$$

In second quantization:

$$\hat{V}_{2B} = \sum_{\substack{p < q \\ r < s}} \langle p q | \hat{V}_{12} | r s \rangle_a a_p^+ a_q^+ a_s^- a_r^-$$

↑
note ordering
↓

$$= \frac{1}{(2!)^2} \sum_{\substack{p, q \\ r, s}} \langle p q | \hat{V}_{12} | r s \rangle_a a_p^+ a_q^+ a_s^- a_r^-$$

Antisymmetrized 2-body matrix elements

$$V_{pqrs} = \langle p q | \hat{V}_{12} | r s \rangle_a$$

anti symmetry means

$$V_{pqrs} = -V_{qprs} = -V_{pqsr} = V_{qpsr}$$

$$\langle_{pq} | V_{12} | rs \rangle_a$$

$$= \left(\frac{1}{\sqrt{2}}\right)^2 \left[\langle_{pq} | \langle_{rs} - \langle_{qr} | \langle_{ps} \right] V_{12}$$

$$[|rs\rangle_1 |s\rangle_2 - |s\rangle_1 |r\rangle_2]$$

use notation $|pq\rangle = |p\rangle_1 |q\rangle_2$

$$= \frac{1}{2} \left[\langle_{pq} | V_{12} | rs \rangle - \langle_{qp} | V_{12} | rs \rangle \right.$$

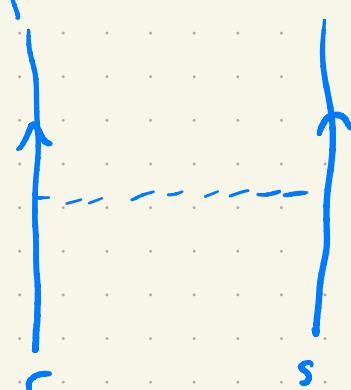
$$\left. - \langle_{pq} | V_{12} | sr \rangle + \langle_{qp} | V_{12} | sr \rangle \right]$$

$$= \langle_{qp} | V_{12} | rs \rangle \quad = \langle_{pq} | V_{12} | rs \rangle$$

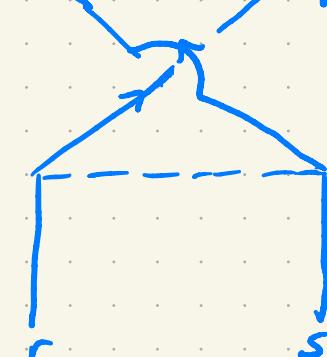
Why? b/c $V_{12} = V_{21}$

$$= \langle_{pq} | V_{12} | rs \rangle - \langle_{qp} | V_{12} | rs \rangle$$

p direct a



p exchange q



*Three-body operators

$$\hat{V}_{3B} = \left(\frac{1}{3!}\right)^2 \sum_{\substack{pqr \\ stu}} V_{pqrstu} a_p^+ a_q^+ a_r^+ a_u a_t a_s$$

↑

matrix elements are antisymmetric
under any exchange of p,q,r
and s,t,u.

Evaluating energy expectation values

Consider $H = H^{1B} + H^{2B}$

$\langle H \rangle$ for a state $|\phi\rangle \leftarrow |p_1 \dots p_A\rangle$

can be evaluated using occupation numbers n_p

$$n_p = \begin{cases} 1 & \text{if } |p\rangle \in \{ |p_1 \dots p_A\rangle \}, \\ 0 & \text{otherwise.} \end{cases}$$

$$\langle H \rangle = \sum_p n_p H_{pp}^{1B} + \frac{1}{2} \sum_{pq} n_p n_q H_{pq}^{2B}$$

Exercise: Derive this starting from

$$|\psi\rangle = a_{p_1}^+ \dots a_{p_A}^+ |0\rangle$$

$$H = \sum_{pq} H_{pq}^{1B} a_p^+ a_q + \frac{1}{4} \sum_{rs} H_{pqrs}^{2B} a_p^+ a_q^+ a_r a_s$$